Reduced density matrices and symmetry breaking with MPS

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Outline

- Monogamy properties of entanglement vs translational invariance
- Convex sets and the geometry of reduced density matrices
- Symmetry breaking and ruled surfaces
Monogamy of Entanglement

- Consider the Heisenberg antiferromagnet on 3 spin \( \frac{1}{2} \)’s:

\[
\mathcal{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1}
\]

- What is the ground state?

\[
\left( | \uparrow \rangle | \downarrow \rangle - | \downarrow \rangle | \uparrow \rangle \right) | \uparrow \rangle
\]

\[
| \uparrow \rangle \left( | \uparrow \rangle | \downarrow \rangle - | \downarrow \rangle | \uparrow \rangle \right)
\]
Monogamy of Entanglement

• Consider the Heisenberg antiferromagnet on 3 spin ½’s:

\[ \mathcal{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \]

• What is the ground state?

\[
\begin{align*}
| \uparrow \rangle (| \uparrow \rangle | \downarrow \rangle - | \downarrow \rangle | \uparrow \rangle ) | \uparrow \rangle & - \\
(\langle \uparrow | \downarrow \rangle - \langle \downarrow | \uparrow \rangle) | \uparrow \rangle &
\end{align*}
\]
Monogamy of Entanglement

• Consider the Heisenberg antiferromagnet on 3 spin ½’s:

\[ \mathcal{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \]

• What is the ground state?

\[
\begin{array}{c}
(\mathbf{\uparrow}\mathbf{\downarrow} - \mathbf{\downarrow}\mathbf{\uparrow}) |\uparrow\rangle - |\downarrow\rangle |\uparrow\rangle \\
\end{array}
\]

• Monogamy: impossibility of sharing a singlet with two spin ½’s
  – Mathematically: there does not exist a density matrix \( \rho_{123} \geq 0 \) which is positive such that its marginals \( \rho_{12} = \text{Tr}_3(\rho_{123}) \) and \( \rho_{23} \) are singlets
  – All interesting long range physics / entanglement in quantum spin systems is a consequence of this optimal trade-off in local marginals
Quantum Marginal Problem

• Chemistry: N-representability
  – Given a set of marginals $\rho_{ij}$, does there exist a global state compatible with it?
    • An efficient algorithm for checking this would immediately lead to an efficient algorithm for finding ground state energies of any Hamiltonian with only 2-body terms
  • Problem in full generality is QMA-hard (quantum NP) -> intractable!
  • For translational invariant cases with nearest neighbor interactions: MPS should allow to solve this problem!

• One case where the marginal problem is solved: mean field theory

  For $i,j=2:N$, $\rho_{1i} = \rho_{1j}$

  – In the limit of infinite N, the only marginals compatible with this symmetry are then ones that are “separable”

    $\rho_{12} = \sum_\alpha p_\alpha \rho_1^\alpha \otimes \rho_2^\alpha$

  – Finite N: de-Finetti theorem

Liu et al. ‘06

Werner ‘89


• Let us get some insight into this frustration by plotting competing terms of the Hamiltonian against each other

  – e.g. Heisenberg XXZ model: competing terms are

\[
\langle X_i X_{i+1} + Y_i Y_{i+1} \rangle \\
\langle Z_i Z_{i+1} \rangle
\]
Scatter plot of all possible reduced density matrices of 2 qubits
Scatter plot of all possible reduced density matrices for translational invariant states in 1 dimension
Scatter plot of all possible reduced density matrices for translational invariant states in 2 dimensions

**singlet**
Scatter plot of all possible reduced density matrices for translational invariant states in infinite dimensions

singlet
Scatter plot of reduced density matrices of 2 qubits
Scatter plot of reduced density matrices of translational invariant systems in 1D
Scatter plot of reduced density matrices of translational invariant systems in infinite dimensions: separable states
Classical spin $\frac{1}{2}$ systems in 2D
Bose Einstein Condensation

\[ |\langle \psi \rangle| \]
\[ \langle \nabla \psi^+ \nabla \psi \rangle \]

Graph showing the relationship between \( |\langle \psi \rangle| \) and \( \langle \nabla \psi^+ \nabla \psi \rangle \) with various lines and a shaded region.